

MISSOURI DEPARTMENT OF NATURAL RESOURCES



CLEANUP LEVELS FOR MISSOURI (CALM) Appendix A

Tier 1 Soil and Groundwater Cleanup Standards

**Division of Air and Land Protection
Hazardous Waste Program**

Revised June 29, 2001

CLEANUP LEVELS FOR MISSOURI (CALM)

APPENDIX A – FORMULAS FOR TIER 1/TIER 2 SOIL TARGET CONCENTRATIONS

PUB468A





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Table A1. CALM Formulas

Formula Description	Formula	Formula Number
<p>Ingestion/dermal contact/inhalation (IDI) pathway soil target concentration (STARC) for noncarcinogenic contaminants, mg/kg</p> <p><i>Note: For scenario "C" calculations, drop terms BW_C, ED_C, IRAC, IRSC, and SAC from the formula</i></p>	$C_{IDI} = \frac{THI * AT_n}{EF * (Ingestion + Inhalation + Dermal)}$ <p>Where:</p> $Ingestion = \left\{ \frac{1}{RfD_o} * 10^{-6} * OAE * \left[\left(\frac{IRS_C * ED_C}{BW_C} \right) + \left(\frac{IRS_A * ED_A}{BW_A} \right) \right] \right\}$ $Inhalation = \left\{ \frac{1}{RfD_i} * \left(\frac{1}{VF} + \frac{1}{PEF} \right) * \left[\left(\frac{IRA_C * ED_C}{BW_C} \right) + \left(\frac{IRA_A * ED_A}{BW_A} \right) \right] \right\}$ $Dermal = \left\{ \frac{1}{RfD_d} * ABS * AF * 10^{-6} * ABS * \left[\left(\frac{SA_C * ED_C}{BW_C} \right) + \left(\frac{SA_A * ED_A}{BW_A} \right) \right] \right\}$	<p>(1)</p>

Table A1. CALM Formulas

Formula Description	Formula	Formula Number
<p>Ingestion/dermal contact/inhalation (IDI) pathway soil target concentration (STARC) for carcinogenic contaminants, mg/kg</p> <p><i>Note: For scenario "C" calculations, drop terms BW_C, ED_C, IRAC, IRSC, and SAC from the formula</i></p>	$C_{IDI} = \frac{TR * AT_c}{EF * (Ingestion + Inhalation + Dermal)}$ <p>Where:</p> $Ingestion = \left\{ SF_o * 10^{-6} * \left[\left(\frac{IRSC * ED_C}{BW_C} \right) + \left(\frac{IRSA * ED_A}{BW_A} \right) \right] \right\}$ $Inhalation = \left\{ SF_i * \left(\frac{1}{VF} + \frac{1}{PEF} \right) * \left[\left(\frac{IRAC * ED_C}{BW_C} \right) + \left(\frac{IRAA * ED_A}{BW_A} \right) \right] \right\}$ $Dermal = \left\{ SF_d * ABS * AF * 10^{-6} * \left[\left(\frac{SAC * ED_C}{BW_C} \right) + \left(\frac{SAA * ED_A}{BW_A} \right) \right] \right\}$	(2)
<p>Particulate emission factor (PEF), m³/kg</p>	$PEF = \frac{Q}{C} * \left[\frac{3600 \frac{sec}{hr}}{0.036 * (1 - v) * \left(\frac{U_m}{U_t} \right)^3 * F(x)} \right]$	(3)
<p>Volatilization factor, m³/kg</p>	$VF = \frac{Q}{C} * \frac{\left(\sqrt{3.14 * D_{app} * T} \right) * 10^{-4} \frac{m^2}{cm^2}}{2 * \rho_b * D_{app}}$	(4)
<p>Apparent diffusivity, cm²/sec</p>	$D_{app} = \frac{\left(\theta_a \right)^{\frac{10}{3}} * D_i * H' + \left(\theta_w \right)^{\frac{10}{3}} * D_w}{n^2 * \left[\left(\rho_b * K_d \right) + \theta_w + \left(\theta_a * H' \right) \right]}$	(5)

Table A1. CALM Formulas

Formula Description	Formula	Formula Number
Soil/water partition coefficient, l/kg	$K_d = f_{oc} * K_{oc} \text{ for organics}$ $K_d = \text{literature-derived value for metals (see Table A4)}$	(6)
Contaminant saturation level in soil, mg/kg	$C_{sat} = \frac{[(K_d * \rho_b) + \theta_w + (H' * \theta_a)] * S}{\rho_b}$	(7)
Leaching to groundwater pathway soil target concentration (C_{leach}) when point of compliance is at the source, mg/kg	$C_{leach} = C_w \left[Kd + \frac{\theta_w + \theta_a * H'}{\rho_b} \right]$	(8)
Contaminant concentration in groundwater directly beneath the soil source, mg/l	$C_w = DF * GTARC$	(9)
Dilution factor, unitless	$DF = 1 + \frac{K * \frac{dh}{dx} * d}{I * L}$	(10)
Mixing zone depth, m Note: should not exceed aquifer thickness (d_a)	$d = \sqrt{0.0112 * L^2 + d_a} \left\{ 1 - \exp \left[\frac{-L * I}{K * \frac{dh}{dx} * d_a} \right] \right\}$	(11)

Table A1. CALM Formulas

Formula Description	Formula	Formula Number
Leaching to groundwater pathway soil target concentration (C_{leach}) when point of compliance is <i>not at the source</i> , mg/kg	$C_{leach} = Cw_{attn} \left[Kd + \frac{\theta_w + \theta_a * H^i}{\rho_b} \right]$ <p>note: for ionizable organics and metals, default Koc and Kd values were used for neutral soil conditions (pH=7)</p>	(12)
Contaminant concentration in groundwater directly beneath the soil source which results in projected (attenuated) groundwater concentration at point of compliance equal to GTARC, mg/l	$Cw_{attn} = \frac{GWTARC}{\left(\frac{C_x}{C_{source}} \right)} * DF$	(13)
Advection/dispersion/degradation factor, unitless	$\frac{C_x}{C_{source}} = \exp \left\{ \frac{x}{2\alpha_x} \left[1 - \sqrt{1 + \frac{4\lambda\alpha_x}{U}} \right] \right\} \operatorname{erf} \left(\frac{S_h}{4\sqrt{\alpha_y x}} \right) \operatorname{erf} \left(\frac{S_v}{2\sqrt{\alpha_z x}} \right)$	(14)
Dispersivity: longitudinal (α_x), transverse (α_y), and vertical (α_z), cm	$\alpha_x = 0.1 * x$ $\alpha_y = \frac{\alpha_x}{3}$ $\alpha_z = \frac{\alpha_x}{20}$	(15)
Contaminant Velocity, cm/day	$U = \frac{K}{\theta_t * R} \frac{dh}{dx} \quad \text{where} \quad R = 1 + \frac{K_d * \rho_b}{\theta_t}$	(16)

Table A1. CALM Formulas

Formula Description	Formula	Formula Number
<p>Mass-limited leaching to groundwater pathway soil target concentration ($C_{leach,ml}$) when point of compliance is <i>at the source</i>, mg/kg</p>	$C_{leach, ml} = \frac{C_w * I * ED}{\rho_b * d_s}$	(17)
<p>Mass-limited leaching to groundwater pathway soil target concentration ($C_{leach,ml}$) when point of compliance is <i>not at the source</i>, mg/kg</p>	$C_{leach, ml} = \frac{C_{w_{attn}} * I * ED}{\rho_b * d_s}$	(18)

Table A2. CALM Formula Parameters and Default Values

Parameter	Definition and Units	Default Values			Can be modified at Tier 2?
		Scenario A	Scenario B	Scenario C	
ABS	Dermal absorption fraction (unitless)	CS	CS	CS	No
AF	Soil to Skin Adherence Factor (mg/cm ²)	1	1	1	No
AT _c	Averaging time for carcinogenic contaminants (days)	25550	25550	25550	No
AT _n	Averaging time for noncarcinogenic contaminants (days)	10950	10950	9125	No
α _x	Longitudinal dispersivity (cm)	SS ¹	SS ¹	SS ¹	Yes
α _y	Transverse dispersivity (cm)	SS ¹	SS ¹	SS ¹	Yes
α _z	Vertical dispersivity (cm)	SS ¹	SS ¹	SS ¹	Yes
BW _a	Body weight for an adult (kg)	70	70	70	No
BW _c	Body weight for a child (kg)	15	15	NA	No
C _{DER}	Soil target concentration for the dermal contact pathway (mg/kg)	CS,SS ¹	CS,SS ¹	CS,SS ¹	Yes
C _{DI}	Soil target concentration for ingestion/dermal contact/inhalation pathway (mg/kg)	CS,SS	CS,SS	CS,SS	Yes
C _{ING}	Soil target concentration for the soil ingestion pathway (mg/kg)	CS,SS ¹	CS,SS ¹	CS,SS ¹	Yes
C _{INH}	Soil target concentration for the inhalation pathway (mg/kg)	CS,SS ¹	CS,SS ¹	CS,SS ¹	Yes
C _{leach}	Soil target concentration for the leaching to groundwater pathway (mg/kg)	CS,SS	CS,SS	CS,SS	Yes
C _{leach,ml}	Mass-limited soil target concentration for the leaching to groundwater pathway (mg/kg)	CS,SS ¹	CS,SS ¹	CS,SS ¹	Yes
C _{sat}	Soil saturation concentration (mg/kg)	CS,SS	CS,SS	CS,SS	Yes
C _w	Unsaturated zone porewater leachate contaminant concentration (mg/l).	CS,SS	CS,SS	CS,SS	Yes
C _{w,attn}	Calculated contaminant concentration in groundwater directly beneath the soil source form when the groundwater point of compliance is not at the source (mg/l).	CS,SS ¹	CS,SS ¹	CS,SS ¹	Yes
C _x /C _{source}	Groundwater contaminant attenuation factor (unitless)	CS,SS ¹	CS,SS ¹	CS,SS ¹	Yes
d	Depth of groundwater mixing zone (m) <i>note: should not exceed aquifer thickness (d_a)</i>	SS ²	SS ²	SS ²	Yes
d _a	Aquifer thickness (m)	SS ²	SS ²	SS ²	Yes
D _{app}	Apparent diffusivity (cm ² /sec)	CS	CS	CS	Yes
DF	Dilution factor (unitless)	20	20	20	Yes
dh/dx	Hydraulic gradient (m/m)	SS ²	SS ²	SS ²	Yes
D _i	Diffusivity in air (cm ² /sec)	CS	CS	CS	No
d _s	Average soil contaminant source depth (m)	SS ¹	SS ¹	SS ¹	Yes
D _w	Diffusivity in water (cm ² /sec)	CS	CS	CS	No
ED _A	Exposure duration for an adult (years)	24	24	25	No
ED _C	Exposure duration for a child (years)	6	6	NA	No
EF	Exposure frequency (days/year)	350	250	250	No

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Table A2. CALM Formula Parameters and Default Values

Parameter	Definition and Units	Default Values			Can be modified at Tier 2?
		Scenario A	Scenario B	Scenario C	
f_{oc}	Fraction of organic carbon in soil (unitless)	0.006	0.006	0.006	Yes
F(x)	Function dependent on U_m/U_i , derived using Cowherd et al. (1985) (unitless)	0.194	0.194	0.194	Yes
GTARC	Groundwater target concentration (mg/l)	CS	CS	CS	No
λ	First order contaminant degradation constant (days)	CS ¹	CS ¹	CS ¹	Yes
H'	Henry's law constant at 25°C (unitless) Note: H'=H*41	CS	CS	CS	No
I	Infiltration rate (m/year)	SS ²	SS ²	SS ²	Yes
IRA _A	Air inhalation rate for an adult (m ³ /day)	20	20	20	No
IRA _C	Air inhalation rate for a child (m ³ /day)	10	10	NA	No
IRS _A	Soil ingestion rate for an adult (mg/day)	100	100	100	No
IRS _C	Soil ingestion rate for a child (mg/day)	200	NA	NA	No
K	Hydraulic conductivity (m/year)	SS ²	SS ²	SS ²	Yes
K _d	Soil-water partition coefficient (L/kg)	CS ³	CS ³	CS ³	Yes
K _{oc}	Soil organic carbon-water partition coefficient (L/kg)	CS ⁴	CS ⁴	CS ⁴	Yes
L	Soil contaminant source length parallel to groundwater flow (m)	SS ¹	SS ¹	SS ¹	Yes
n	Total soil porosity (L _{pore} /L _{soil})	0.434	0.434	0.434	Yes
OAE	Oral Absorption Efficiency (unitless)	CS	CS	CS	No
PEF	Particulate Emission Factor (m ³ /kg)	1.32x10 ⁹	1.32x10 ⁹	1.32x10 ⁹	Yes
ρ_b	Soil dry bulk density (kg/L)	1.5	1.5	1.5	Yes
Q/C	Inverse of mean contaminant concentration at center of a 0.5 acre square source $\left(\frac{g}{m^2 \cdot sec} / \frac{kg}{m^3} \right)$	81.64	81.64	81.64	No
RfD _d	Dermal contact chronic reference dose (mg/kg-day)	CS	CS	CS	No
RfD _i	Ingestion chronic reference dose (mg/kg-day)	CS	CS	CS	No
RfD _o	Inhalation chronic reference dose (mg/kg-day)	CS	CS	CS	No
S	Contaminant solubility in water at 25°C (mg/L)	CS	CS	CS	No
S _h	Soil contaminant source width perpendicular to groundwater flow in the <i>horizontal</i> plane (m)	SS ¹	SS ¹	SS ¹	Yes
S _v	Soil contaminant source width perpendicular to groundwater flow in the <i>vertical</i> plane (m)	SS ¹	SS ¹	SS ¹	Yes
SA _A	Skin surface area for an adult (cm ²)	4714	4714	4714	No
SA _C	Skin surface area for a child (cm ²)	4236	4236	NA	No
SF _d	Carcinogenic dermal contact slope factor (mg/kg-day)	CS	CS	CS	No
SF _i	Carcinogenic inhalation slope factor (mg/kg-day)	CS	CS	CS	No
SF _o	Carcinogenic ingestion slope factor (mg/kg-day)	CS	CS	CS	No
T	Exposure interval (sec)	9.5x10 ⁸	9.5x10 ⁸	7.9x10 ⁸	No
THI	Target hazard index (unitless)	1	1	1	No

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Table A2. CALM Formula Parameters and Default Values

Parameter	Definition and Units	Default Values			Can be modified at Tier 2?
		Scenario A	Scenario B	Scenario C	
TR	Target cancer risk (unitless)	10 ⁻⁵	10 ⁻³	10 ⁻³	No
θ_w	Water-filled soil porosity (L _{water} /L _{soil})	0.15	0.15	0.15	Yes
θ_a	Air-filled soil porosity (L _{air} /L _{soil})	0.28	0.28	0.28	Yes
U	Linear average groundwater (or seepage) velocity (cm/day)	SS ¹	SS ¹	SS ¹	Yes
U _m	Mean annual wind speed (m/sec)	4.69	4.69	4.69	Yes
U _t	Equivalent threshold value of windspeed at 7m (m/sec)	11.32	11.32	11.32	Yes
V	Fraction of vegetative cover at the site (unitless)	0.5	0.5	0.5	Yes
VF	Volatilization factor (m ³ /kg)	CS,SS	CS,SS	CS,SS	Yes
x	Centerline distance from downgradient edge of soil source to point of compliance, x is in the direction of groundwater flow (m)	SS ¹	SS ¹	SS ¹	Yes

SS = Site specific value

CS = Chemical specific value

NA = Not applicable

1. Parameter is only relevant at Tier 2 evaluation.
2. Parameter used to calculate dilution factor (DF). Since a default of 20 is used for DF at Tier 1, this parameter is only relevant at Tier 2 where a site-specific value is used.
3. For metals, K_d values were selected for neutral soil conditions (pH=7.0).
4. For ionizable organic contaminants, K_{oc} values were selected for neutral soil conditions (pH=7.0).

Figure A1. Simplifying Assumptions For The Soil Leaching To Groundwater Pathway Equation (C_{leach})

- Unconfined saturated zone with homogeneous and isotropic hydrologic properties.
- Infinite soil contaminant source (i.e. steady-state soil contaminant concentrations are maintained over the entire 30 year exposure period). Note: this assumption is not made when using the mass-limited leaching formula ($C_{leach,ml}$, see Table A1. Formula #s 17 and 18).
- Uniformly distributed soil contamination from the soil surface to the top of the saturated zone.
- Groundwater directly beneath the soil contaminant source could potentially be utilized as drinking water
- Instantaneous and linear equilibrium soil/water and organic carbon/water partitioning.
- No contaminant attenuation (i.e. microbial or chemical degradation, or sorption,) in the saturated zone directly below the soil contaminant source(s).
- No non-aqueous phase liquids (NAPLs) present.

Figure A2. Simplifying Assumptions For The Advection-Dispersion-Degradation Equation (C_x/C_{source})

- Unconfined saturated zone with homogeneous and isotropic hydrologic properties.
- Infinite soil contaminant source (i.e. steady-state soil contaminant concentrations are maintained over the entire exposure period).
- No contaminant sorption or volatilization losses in saturated zone
- Contaminant degradation (microbial and chemical) in the saturated zone is described by a first order degradation constant
- No non-aqueous phase liquids (NAPLs) are present.

Figure A3. Summary Of Formula Parameters Which May Be Modified At Tier 2 Using Site-Specific Information

Site-Specific Variables Which May Be Measured In The Field	<p>α_x Longitudinal dispersivity (cm)</p> <p>α_y Transverse dispersivity (cm)</p> <p>α_z Vertical dispersivity (cm)</p> <p>d_a Aquifer thickness (m)</p> <p>dh/dx Hydraulic gradient (m/m)</p> <p>d_s Average soil contaminant source depth (m)</p> <p>f_{oc} Fraction of organic carbon in soil (unitless)</p> <p>λ First order contaminant degradation constant (days)</p> <p>I Infiltration rate (m/year)</p> <p>K Hydraulic conductivity (m/year)</p> <p>L Soil contaminant source length parallel to groundwater flow (m)</p> <p>n Total soil porosity (L_{pore}/L_{soil})</p> <p>ρ_b Soil dry bulk density (kg/L)</p> <p>S_h Soil contaminant source width perpendicular to groundwater flow in the <i>horizontal</i> plane (m)</p> <p>S_v Soil contaminant source width perpendicular to groundwater flow in the <i>vertical</i> plane (m)</p> <p>θ_w Water-filled soil porosity (L_{water}/L_{soil})</p> <p>θ_a Air-filled soil porosity (L_{air}/L_{soil})</p> <p>U_m Mean annual wind speed (m/sec)</p> <p>U_t Equivalent threshold value of windspeed at 7m (m/sec)</p> <p>V Fraction of vegetative cover at the site (unitless)</p> <p>x Centerline distance from downgradient edge of soil source to point of compliance, x is in the direction of groundwater flow (m)</p>
Calculated Site-Specific Variables	<p>C_{IDI} Soil target concentration for ingestion/dermal contact/inhalation pathway (mg/kg)</p> <p>C_{ING} Soil target concentration for the soil ingestion pathway (mg/kg)</p> <p>C_{INH} Soil target concentration for the inhalation pathway (mg/kg)</p> <p>C_{leach} Soil target concentration for the leaching to groundwater pathway (mg/kg)</p> <p>$C_{leach, ml}$ Mass-limited soil target concentration for the leaching to groundwater pathway (mg/kg)</p>

Figure A3 (cont.) Summary of Formula Parameters Which May Be Modified At Tier 2 Using Site-Specific Information

Calculated Site-Specific Variables	C_{sat}	Soil saturation concentration (mg/kg)
	C_w	Calculated contaminant concentration in groundwater directly beneath the soil source for when the groundwater point of compliance is at the source (mg/l).
	$C_{w_{attn}}$	Calculated contaminant concentration in groundwater directly beneath the soil source form when the groundwater point of compliance is not at the source (mg/l).
	C_x/C_{source}	Groundwater contaminant attenuation factor (unitless)
	D	Depth of mixing zone (m)
	D_{app}	Apparent diffusivity (cm ² /sec)
	DF	Dilution factor (unitless)
	F(x)	Function dependent on U_m/U_t , derived using Cowherd et al. (1985) (unitless)
	K_d	Soil-water partition coefficient (L/kg)
	PEF	Particulate emission factor (m ³ /kg)
	U	Linear average groundwater (or seepage) velocity (cm/day)
	VF	Volatilization factor (m ³ /kg)

Table A3. Toxicological Values

Chemicals	CAS #	Noncarcinogenic Tox Values				Carcinogenic Tox Values					Dermal Values	
		RfDo	RfC	RfDi	RfDd	Class	SFo	URi	SFi	SFd	OAE	ABS
		mg/kg-d	mg/m ³	mg/kg-d	mg/kg-d		(mg/kg-d) ⁻¹	(ug/m ³) ⁻¹	(mg/kg-d) ⁻¹	(mg/kg-d) ⁻¹	unitless	unitless
Acenaphthene	83-32-9	0.06			0.06					1	0.3	
Acetone	67-64-1	0.1			0.095	D				0.95	0.3	
Acetonitrile	75-05-8	0.006	0.06	0.017	0.006	D				1	0.3	
Acifluorfen	62476-59-9	0.013			0.013		0.013		0.013	1	0.3	
Acrylamide	79-06-1	0.0002			0.0002	B2	4.5	0.0013	4.55	4.5	1	0.1
Acrylic Acid	79-10-7	0.5	0.001	0.00029	0.5					1	0.1	
Acrylonitrile	107-13-1	0.001	0.002	0.001	0.001	B1	0.54	0.000068	0.238	0.54	1	0.3
Alachlor	15972-60-8	0.01			0.01	B2	0.08			0.08	1	0.1
Aldicarb	116-06-3	0.001			0.001	D				1	0.1	
Aldicarb sulfone	1646-88-4	0.001			0.001					1	0.1	
Aldrin	309-00-2	0.00003			0.00003	B2	17	0.004857	16.9995	17	1	0.1
Allyl alcohol	107-18-6	0.005			0.005					1	0.1	
Allyl chloride	107-05-1	0.05	0.001	0.00029	0.05	C				1	0.1	
Ametryn	834-12-8	0.009			0.009					1	0.1	
Ammonium sulfamate	7773-06-0	0.2			0.2					1	0.3	
Anthracene	120-12-7	0.3			0.3	D				1	0.3	
Antimony	7440-36-0	0.0004	0.0002	5.7E-05	0.0004	B1				1	0.01	
Arsenic	7440-38-2	0.0003				A	1.50	0.0043		0.95	0.001	
Atrazine	1912-24-9	0.035			0.035	C	0.222			0.222	1	0.1
Barium	7440-39-3	0.07	0.0005	0.00014	0.07	D				1	0.01	
Baygon	114-26-1	0.004			0.004					1	0.1	
Bentazon	25057-89-0	0.0025			0.0025	E				1	0.1	
Benzene	71-43-2	0.003	0.006	0.00171	0.003	A	0.029	0.0000083	0.02905	0.029	1	0.3
Benzidine	92-87-5	0.003			0.003	A	230	0.067	234.5	230	1	0.1
Benzo[a]anthracene	56-55-3					B2				1	0.13	
Benzo(a)pyrene	50-32-8					B2	7.3	0.00174	6.09	8.58824	0.85	0.13
Benzo[b]fluoranthene	205-99-2					B2				1	0.13	
Benzo[k]fluoranthene	207-08-9					B2				1	0.13	
Benzoic Acid	65-85-0	4			4	D				1	0.1	
Beryllium	7440-41-7	0.002	0.02	0.00571	0.00002	B1	4.3	0.0024	8.4	430	0.01	0.01
1,1-Biphenyl	92-52-4	0.05			0.05	D				1	0.3	
Bis(2-ethylhexyl)phthalate	117-81-7	0.02			0.02	B2	0.014			0.014	1	0.004
Bis(2-chloroethyl) ether	111-44-4					B2	1.1	0.00033	1.155	1.1	1	0.3
Bis(2-chloroisopropyl) ether	39638-32-9	0.04			0.04		0.07	0.00001	0.035	0.07	1	0.3
Bis (chloromethyl) ether	542-88-1					A	220	0.062	217	220	1	0.3
Boron	7440-42-8	0.09	0.02	0.00571	0.09					1	0.01	
Bromodichloromethane	75-27-4	0.02			0.02	B2	0.062			0.062	1	0.3
Bromoform	75-25-2	0.02			0.02	B2	0.0079	1.14E-06	0.00399	0.0079	1	0.1
4-Bromophenyl phenyl ether	101-55-3					D				1	0.1	

Table A3. Toxicological Values

Chemicals	CAS #	Noncarcinogenic Tox Values				Carcinogenic Tox Values					Dermal Values	
		RfDo	RfC	RfDi	RfDd	Class	SFo	URi	SFi	SFd	OAE	ABS
		mg/kg-d	mg/m ³	mg/kg-d	mg/kg-d		(mg/kg-d) ⁻¹	(ug/m ³) ⁻¹	(mg/kg-d) ⁻¹	(mg/kg-d) ⁻¹	unitless	unitless
Butyl benzyl phthalate	85-68-7	0.2			0.2	C					1	0.1
Cadmium	7440-43-9	0.0005			0.0005	B1		0.0018	6.3		1	0.01
Captan	133-06-2	0.13			0.13	B2	0.0035			0.0035	1	0.1
Carbaryl	63-25-2	0.1			0.10	D					1	0.1
Carbazole	86-74-8					B2	0.02			0.02	1	0.1
Carbofuran	1563-66-2	0.005			0.005						1	0.1
Carbon disulfide	75-15-0	0.1	0.7	0.2	0.1	D					1	0.3
Carbon tetrachloride	56-23-5	0.0007	0.002	0.00057	0.0007	B2	0.13	0.000015	0.0525	0.13	1	0.3
Carboxin	5234-68-4	0.1			0.1						1	0.1
Chloramben	133-90-4	0.015			0.015						1	0.1
Chlordane	12789-03-6	0.0005	0.0007	0.0002	0.0004	B2	0.35	0.0001	0.35	0.4375	0.8	0.04
p-Chloroaniline	106-47-8	0.004			0.004						1	0.1
Chlorobenzene	108-90-7	0.02	0.06	0.01714	0.0026	D					0.13	0.3
Chloroform	67-66-3	0.01	0.0003	8.6E-05	0.01	B2	0.0061	0.000023	0.0805	0.0061	1	0.3
2-Chlorophenol	95-57-8	0.005			0.005						1	0.3
Chlorothalonil	1897-45-6	0.015			0.015	B2	0.011			0.011	1	0.1
Chlorpyrifos	2921-88-2	0.003			0.003						1	0.1
Chromium(VI)	18540-29-9	0.003	8E-06			A		0.012			0.025	0.01
Chrysene	218-01-9					B2					1	0.13
Copper	7440-50-8					D					1	0.01
Cyanazine	21725-46-2	0.002			0.002	C	0.84			0.84	1	0.1
Cyanide, free	57-12-5	0.02									1	
Cyanogen bromide	506-68-3	0.09			0.09						1	0.3
Dalapon, sodium salt	75-99-0	0.03			0.03						1	0.1
2,4-Dichlorophenoxyacetic acid (2,4-D)	94-75-7	0.01			0.009						0.9	0.05
DDD	72-54-8					B2	0.24			0.34286	0.7	0.03
DDE	72-55-9					B2	0.34			0.48571	0.7	0.03
DDT	50-29-3	0.0005			0.00035	B2	0.34	0.000097	0.3395	0.48571	0.7	0.03
Demeton	8065-48-3	0.00004			0.00004						1	0.3
Diazinon	333-41-5	0.0009			0.0009						1	0.1
Dibenz[a,h]anthracene	53-70-3					B2					1	0.13
Dibenzofuran	132-64-9	0.004			0.004	D					1	0.3
1,4-Dibromobenzene	106-37-6	0.01			0.01						1	0.1
Dibromochloromethane	124-48-1	0.02			0.02	C	0.084			0.084	1	0.1
1,2-Dibromo-3-chloropropane	96-12-8		0.0002	5.7E-05		B2	1.4	6.86E-07	0.0024	1.4	1	0.1
Dibutyl phthalate	84-74-2	0.1			0.1	D					1	0.1
Dicamba	1918-00-9	0.03			0.03						1	0.1
1,2-Dichlorobenzene	95-50-1	0.09	0.2	0.05714	0.045	D					0.5	0.3

Table A3. Toxicological Values

Chemicals	CAS #	Noncarcinogenic Tox Values				Carcinogenic Tox Values					Dermal Values	
		RfDo	RfC	RfDi	RfDd	Class	SFo	URi	SFi	SFd	OAE	ABS
		mg/kg-d	mg/m ³	mg/kg-d	mg/kg-d		(mg/kg-d) ⁻¹	(ug/m ³) ⁻¹	(mg/kg-d) ⁻¹	(mg/kg-d) ⁻¹	unitless	unitless
1,4-Dichlorobenzene	106-46-7	0.03	0.8	0.22857	0.03	C	0.024	6.285E-06	0.022	0.024	1	0.3
3,3-Dichlorobenzidine	91-94-1					B2	0.45			0.45	1	0.1
1,2-Dichloroethane	107-06-2	0.03	0.005	0.00143	0.030	B2	0.091	0.000026	0.091	0.091	1	0.3
1,1-Dichloroethylene	75-35-4	0.009			0.009	C	0.6	0.00005	0.175	0.6	1	0.3
cis-1,2-Dichloroethylene	156-59-2	0.01			0.01	D					1	0.03
trans-1,2-Dichloroethylene	156-60-5	0.02			0.02						1	0.03
2,4-Dichlorophenol	120-83-2	0.003			0.003						1	0.1
4-(2,4-Dichlorophenoxy) butyric acid (2,4-DB)	94-82-6	0.008			0.008						1	0.1
1,2-Dichloropropane	78-87-5		0.004	0.00114		B2	0.068			0.068	1	0.3
1,3-Dichloropropene	542-75-6	0.0003	0.02	0.00571	0.0003	B2	0.18	0.000037	0.1295	0.18	1	0.3
Dieldrin	60-57-1	0.00005			0.00005	B2	16	0.00457	15.995	16	1	0.1
Diethyl phthalate	84-66-2	0.8			0.8	D					1	0.1
Dimethoate	60-51-5	0.0002			0.0002						1	0.1
Dimethyl phthalate	131-11-3	10			10	D					1	0.1
2,4-Dimethylphenol	105-67-9	0.02			0.02						1	0.1
2,6-Dimethylphenol	576-26-1	0.0006			0.0006						1	0.1
3,4-Dimethylphenol	95-65-8	0.001			0.001						1	0.1
1,3-Dinitrobenzene	99-65-0	0.0001			0.0001	D					1	0.1
2,4-Dinitrophenol	51-28-5	0.002			0.002	B2					1	0.1
2,4-Dinitrotoluene	121-14-2	0.002			0.002	B2	0.68			0.68	1	0.1
2,6-Dinitrotoluene	606-20-2	0.001			0.001	B2	0.68			0.68	1	0.1
Di-n-octylphthalate	117-84-0	0.02			0.02						1	0.1
Dinoseb	88-85-7	0.001			0.001	D					1	0.1
1,4-Dioxane	123-91-1					B2	0.011			0.011	1	0.1
Diphenamid	957-51-7	0.03			0.03						1	0.1
Diphenylamine	122-39-4	0.025			0.025	D					1	0.1
Diquat	85-00-7	0.0022			0.0022						1	0.1
Disulfoton	298-04-4	0.00004			0.00004						1	0.1
Diuron	330-54-1	0.002			0.002						1	0.1
Endosulfan	115-29-7	0.006			0.006						1	0.1
Endothall	145-73-3	0.02			0.02						1	0.1
Endrin	72-20-8	0.0003			0.0003	D					1	0.1
Ethylbenzene	100-41-4	0.1	1	0.28571	0.092	D					0.92	0.3
Ethylene glycol	107-21-1	2			2	D					1	0.1
Ethylene thiourea	96-45-7	0.00008			0.00008	B2	0.11			0.11	1	0.1
Fenamiphos	22224-92-6	0.00025			0.00025						1	0.1
Fluometuron	2164-17-2	0.013			0.013						1	0.1
Fluoranthene (PAH)	206-44-0	0.04			0.02	D					0.5	0.1

Table A3. Toxicological Values

Chemicals	CAS #	Noncarcinogenic Tox Values				Carcinogenic Tox Values					Dermal Values	
		RfDo	RfC	RfDi	RfDd	Class	SFo	URi	SFi	SFd	OAE	ABS
		mg/kg-d	mg/m ³	mg/kg-d	mg/kg-d		(mg/kg-d) ⁻¹	(ug/m ³) ⁻¹	(mg/kg-d) ⁻¹	(mg/kg-d) ⁻¹	unitless	unitless
Fluorene (PAH)	86-73-7	0.04			0.04	D					1	0.3
Fonofos	944-22-9	0.02			0.02						1	0.1
Formaldehyde	50-00-0	0.2			0.2	B1		0.000013	0.0455		1	0.1
Glyphosate	1071-83-6	0.1			0.1	D					1	0.1
Heptachlor	76-44-8	0.0005			0.0005	B2	4.5	0.0013	4.55	4.5	1	0.1
Heptachlor epoxide	1024-57-3	1.3E-05			1.3E-05	B2	9.1	0.0026	9.1	9.1	1	0.1
Hexachlorobenzene	118-74-1	0.0008			0.0008	B2	1.6	0.00046	1.61	1.6	1	0.1
Hexachlorobutadiene	87-68-3	0.0002			0.0002	C	0.078	0.000022	0.077	0.078	1	0.1
a-Hexachlorocyclohexane	319-84-6					B2	6.3	0.0018	6.3	6.3	1	0.1
b-Hexachlorocyclohexane	319-85-7					C	1.8	0.0005145	1.80075	1.8	1	0.1
g-Hexachlorocyclohexane	58-89-9	0.0003			0.0003	B2-C	1.3			1.3	1	0.1
d-Hexachlorocyclohexane	319-86-8										1	0.1
Hexachlorocyclopentadiene	77-47-4	0.007	0.00007	0.00002	0.007	D					1	0.1
Hexachloroethane	67-72-1	0.001			0.001	C	0.014	0.000004	0.014	0.014	1	0.1
Hexachlorophene	70-30-4	0.0003			0.0003						1	0.1
n-Hexane	110-54-3	0.06	0.2	0.05714	0.06						1	0.3
Hexazinone	51235-04-2	0.033			0.033						1	0.1
HMX	2691-41-0	0.05			0.05	D					1	0.1
Indeno[1,2,3-cd]pyrene	193-39-5					B2					1	0.13
Isophorone	78-59-1	0.2			0.2	C	0.00095			0.00095	1	0.1
Isopropylbenzene	98-82-8	0.1	0.4	0.11429	0.1	D					1	0.3
Lead	7439-92-1					B2						
Malathion	121-75-5	0.02			0.02						1	0.1
Maleic anhydride	108-31-6	0.1			0.1						1	0.1
Maleic hydrazide	123-33-1	0.5			0.5						1	0.1
Maneb	12427-38-2	0.005			0.005		0.06			0.06	1	0.1
Manganese	7439-96-5	0.14	0.00005	1.4E-05	0.14	D					1	0.3
Mercury	7439-97-6	0.0003	0.0003	8.6E-05	4.5E-05	D					0.15	0.001
Methamidophos	10265-92-6	0.00005			0.00005						1	0.1
Methanol	67-56-1	0.5			0.5						1	0.1
Methomyl	16752-77-5	0.025			0.025						1	0.1
Methoxychlor	72-43-5	0.005			0.005	D					1	0.1
2-Methyl-4-chlorophenoxyacetic acid (MCPA)	94-74-6	0.0005			0.0005						1	0.1
Methyl ethyl ketone	78-93-3	0.6	1	0.28571	0.6	D					1	0.3
Methyl iodide	74-88-4					C					1	0.3
Methyl isobutyl ketone	108-10-1	0.08	0.08	0.02286	0.08	D					1	0.3
Methyl parathion	298-00-0	0.00025			0.00025						1	0.1
2-Methylphenol	95-48-7	0.05			0.05	C					1	0.1

Table A3. Toxicological Values

Chemicals	CAS #	Noncarcinogenic Tox Values				Carcinogenic Tox Values					Dermal Values	
		RfDo	RfC	RfDi	RfDd	Class	SFo	URi	SFi	SFd	OAE	ABS
		mg/kg-d	mg/m ³	mg/kg-d	mg/kg-d		(mg/kg-d) ⁻¹	(ug/m ³) ⁻¹	(mg/kg-d) ⁻¹	(mg/kg-d) ⁻¹	unitless	unitless
3-Methylphenol	108-39-4	0.05			0.05	C					1	0.1
4-Methylphenol	106-44-5	0.005			0.00325	C					0.65	0.1
Methylene chloride	75-09-2	0.06	3	0.85714	0.06	B2	0.0075	4.7E-07	0.00165	0.0075	1	0.3
Methyl tert butyl ether (MTBE)	1634-04-4		3								1	0.3
Metolachlor	51218-45-2	0.15			0.15	C					1	0.1
Metribuzin	21087-64-9	0.025			0.025	D					1	0.1
Mirex	2385-85-5	0.0002			0.0002	B2	1.8			1.8	1	0.1
Molybdenum	7439-98-7	0.005			0.005						1	0.001
Naled	300-76-5	0.002			0.002						1	0.1
Naphthalene	91-20-3	0.02	0.003	0.00086	0.0168	D					0.84	0.3
Nickel	7440-02-0	0.02			0.002	A		0.00024	0.84		0.1	0.0005
Nitrobenzene	98-95-3	0.0005	0.002	0.00057	0.0005	D					1	0.3
n-Nitrosodimethylamine	62-75-9					B2	51	0.014	49	51	1	0.1
n-Nitrosodiphenylamine	86-30-6					B2	0.0049			0.0049	1	0.1
Oxamyl	23135-22-0	0.025			0.025						1	0.1
Paraquat	4685-14-7	0.0045			0.0045	C					1	0.1
Pendimethalin	40487-42-1	0.04			0.04						1	0.1
Pentachlorobenzene	608-93-5	0.0008			0.0008	D					1	0.1
Pentachloronitrobenzene	82-68-8	0.003			0.003		0.26			0.26	1	0.1
Pentachlorophenol	87-86-5	0.03			0.03	B2	0.12			0.12	1	0.25
Phenol	108-95-2	0.6			0.57	D					0.95	1
m-Phenylenediamine	108-45-2	0.006			0.006						1	0.1
Phenylmercuric acetate	62-38-4	0.00008			0.00008						1	0.1
Phorate	298-02-2	0.0002			0.0002						1	0.1
Picloram	1918-02-1	0.07			0.07						1	0.1
Polychlorinated biphenyls (PCBs)	1336-36-3	0.00002				B2					1	0.14
Prometon	1610-18-0	0.015			0.015						1	0.1
Pronamide	23950-58-5	0.075			0.075						1	0.1
Propachlor	1918-16-7	0.013			0.013						1	0.1
Propanil	709-98-8	0.005			0.005						1	0.1
Propazine	139-40-2	0.02			0.02						1	0.1
Propham	122-42-9	0.02			0.02						1	0.1
n-Propylbenzene	103-65-1	0.001			0.001						1	0.3
Pyrene (PAH)	129-00-0	0.03			0.03	D					1	0.1
RDX	121-82-4	0.003			0.003		0.11			0.11	1	0.1
Rotenone	83-79-4	0.004			0.004						1	0.1
Selenium	7782-49-2	0.005			0.004	D					0.8	0.1
Silver	7440-22-4	0.005			0.005	D					1	0.3
Silvex	93-72-1	0.008			0.008	D					1	0.1

Table A3. Toxicological Values

Chemicals	CAS #	Noncarcinogenic Tox Values				Carcinogenic Tox Values					Dermal Values	
		RfDo	RfC	RfDi	RfDd	Class	SFo	URi	SFi	SFd	OAE	ABS
		mg/kg-d	mg/m ³	mg/kg-d	mg/kg-d		(mg/kg-d) ⁻¹	(ug/m ³) ⁻¹	(mg/kg-d) ⁻¹	(mg/kg-d) ⁻¹	unitless	unitless
Simazine	122-34-9	0.005			0.005	C	0.12			0.12	1	0.1
Strontium	7440-24-6	0.6			0.6						1	0.01
Strychnine	57-24-9	0.0003			0.0003						1	0.1
Styrene	100-42-5	0.2	1	0.28571	0.2	C					1	0.3
Terbacil	5902-51-2	0.013			0.013						1	0.1
Terbufos	13071-79-9	2.5E-05			2.5E-05						1	0.1
1,1,1,2-Tetrachloroethane	630-20-6	0.03			0.03	C	0.026	0.0000074	0.0259	0.026	1	0.3
1,1,1,2-Tetrachloroethane	79-34-5	0.06			0.042	C	0.2	0.000058	0.203	0.28571	0.7	0.3
Tetrachloroethylene	127-18-4	0.01	0.4	0.11429	0.01	C-B2	0.052	5.8E-07	0.00203	0.052	1	0.03
Tetrahydrofuran	109-99-9	0.18	0.3	0.08571	0.18	C	0.0076	1.942E-06	0.0068	0.0076	1	0.3
Thallium compounds		0.00008			0.00008	D					1	0.01
Toluene	108-88-3	0.2	0.4	0.11429	0.2	D					1	0.03
Toxaphene	8001-35-2					B2	1.1	0.00032	1.12	1.1	1	0.1
Triallate	2303-17-5	0.013			0.013						1	0.1
1,2,4-Trichlorobenzene	120-82-1	0.01	0.2	0.05714	0.01	D					1	0.3
1,3,5-Trichlorobenzene	108-70-3										1	0.3
1,1,1-Trichloroethane	71-55-6	0.02	1	0.28571	0.02	D					1	0.0005
1,1,2-Trichloroethane	79-00-5	0.004			0.004	C	0.057	0.000016	0.056	0.057	1	0.3
Trichloroethylene	79-01-6	0.006			0.006	C-B2	0.011	0.0000017	0.00595	0.011	1	0.0005
Trichlorofluoromethane	75-69-4	0.3	0.7	0.2	0.3						1	0.3
2,4,5-Trichlorophenol	95-95-4	0.1			0.1	D					1	0.1
2,4,6-Trichlorophenol	88-06-2					B2	0.011	0.0000031	0.01085	0.011	1	0.1
1,2,3-Trichloropropane	96-18-4	0.006			0.006		7			7	1	0.3
1,1,2-Trichlorotrifluoroethane	76-13-1	30	30.1	8.6	30						1	0.3
Trifluralin	1582-09-8	0.0075			0.0075	C	0.0077			0.0077	1	0.1
1,2,4-Trimethylbenzene	95-63-6	0.05	0.00595	0.0017	0.05						1	0.3
1,3,5-Trimethylbenzene	108-67-8	0.05	0.006	0.00171	0.05						1	0.3
1,3,5-Trinitrobenzene	99-35-4	0.03			0.03						1	0.1
2,4,6-Trinitrotoluene	118-96-7	0.0005			0.0005	C	0.03			0.03	1	0.1
Vanadium	7440-62-2	0.007			0.007						1	0.01
Vinyl chloride	75-01-4					A	1.9	0.0000844	0.2954	1.9	1	0.0003
Warfarin	81-81-2	0.0003			0.0003						1	0.1
White phosphorus	7723-14-0	0.00002			0.00002	D					1	0.01
Xylenes	1330-20-7	2	0.7	0.2		D					0.92	0.3
Zinc	7440-66-6	0.3			0.075	D					0.25	0.01

Table A4. Chemical Property Values

Chemicals	CAS #	Di cm ² /sec	HLC atm- m ³ /mol	H' unitless	Melting Point (C)	Dw cm ² /sec	Koc cm ³ /g	Kd L/kg	Water Solubility mg/L	GTARC mg/L	Mol. Wt.	Csat mg/kg
Acenaphthene	83-32-9	4.21E-02	1.55E-04	0.006355	93.4	7.69E-06	7080	42.48	4.24	1.2	154.21	
Acetone	67-64-1	1.24E-01	3.88E-05	0.001591	-94.8	1.14E-05	0.575	0.00345	1000000		58.08	103746.9
Acetonitrile	75-05-8	1.30E-01	3.45E-05	0.001415	-45	1.70E-05	15.6	0.0936	1000000		41.05	193864
Acifluorfen	62476-59-9				142				250000	0.001	361.7	
Acrylamide	79-06-1		1.00E-09	4.1E-08	84.5		50	0.3	640000	0.00001	71.08	
Acrylic Acid	79-10-7		1.17E-07	4.8E-06	13.5				1000000		72.06	
Acrylonitrile	107-13-1	1.08E-01	1.38E-04	0.005658	-83.55	1.34E-05	0.85	0.0051	74500	0.00006	53.06	7908.634
Alachlor	15972-60-8		8.32E-09	3.41E-07	40.5		191	1.146	240	0.002	269.5	
Aldicarb	116-06-3		1.44E-09	5.9E-08	99		16	0.096	6030	0.007	190.27	
Aldicarb sulfone	1646-88-4		3.37E-09	1.38E-07	141		3	0.018	7800	0.007	222.26	
Aldrin	309-00-2	1.32E-02	1.70E-04	0.00697	104	4.86E-06	2450000	14700	0.18	0.000002	364.92	
Allyl alcohol	107-18-6		4.99E-06	0.000205	-129		29.5	0.177	317000		58.08	87821.11
Allyl chloride	107-05-1		7.61E-07	3.12E-05	-67		50	0.3	1000000		80.51	400005.8
Ametryn	834-12-8		4.58E-09	1.88E-07	88.5		389	2.334	185	0.06	227.33	
Ammonium sulfamate	7773-06-0				131				684000	2	114.14	
Anthracene	120-12-7	3.24E-02	0.00072	0.029520	215	7.74E-06	29500	177	0.0434	9.6	178.24	
Antimony	7440-36-0				332.2					0.006	121.75	
Arsenic	7440-38-2				814					0.05		
Atrazine	1912-24-9		4.47E-09	1.83E-07	172.5		489	2.934	28	0.003	215.69	
Barium	7440-39-3				385					2		
Baygon	114-26-1		4.00E-07	1.64E-05	91.5		160	0.96	1860	0.003	209.25	
Bentazon	25057-89-0		2.18E-09	8.94E-08	138				50	0.2	240.28	
Benzene	71-43-2	8.80E-02	5.55E-03	0.228	5.5	9.80E-06	58.9	0.3534	1750	0.005	78.11	867.783
Benidine	92-87-5		3.88E-11	1.59E-09	120		174000	1044	322	0.00000012	184.24	
Benzo[a]anthracene	56-55-3	5.10E-02	3.35E-06	1.37E-04	84	9.00E-06	3.98E+05		9.40E-03	0.0000044	228.3	
Benzo(a)pyrene	50-32-8	4.30E-02	1.13E-06	4.63E-05	176.5	9.00E-06	1020000	6120	0.00162	0.0002	252.32	
Benzo[b]fluoranthene	205-99-2	2.26E-02	1.11E-04	4.55E-03	168	5.56E-06	1.23E+06		1.50E-03	0.0000044	252.32	
Benzo[k]fluoranthene	207-08-9	2.26E-02	8.29E-07	3.40E-05	217	5.56E-06	1.23E+06		8.00E-04	0.0000044	252.32	
Benzoic Acid	65-85-0	5.36E-02	1.54E-06	6.31E-05	122.4	7.97E-06	0.6	0.0036	3500		122.12	
Beryllium	7440-41-7				692.2					0.004		
1,1-Biphenyl	92-52-4	4.04E-02	4.08E-04	0.016728	70	8.20E-06	1400	8.4	6.94		154.21	
Bis(2-ethylhexyl)phthalate	117-81-7	3.51E-02	1.02E-07	4.18E-06	-55	3.66E-06	15100000	90600	0.34	0.006	390.57	30804.03
Bis(2-chloroethyl) ether	111-44-4	6.90E-02	1.80E-05	0.000738	-51.9	7.53E-06	15.5	0.093	17200	0.00003	143.01	3321.969
Bis(2-chloroisopropyl) ether	39638-32-9	6.31E-02	1.13E-04	0.004633	-97	6.40E-06	57	0.342	1700	0.3	171.07	752.8702
Bis (chloromethyl) ether	542-88-1	8.87E-02	2.06E-04	0.008446	-41.5	9.40E-06	1.2	0.0072	22000	0.00000016	114.96	2393.085
Boron	7440-42-8				1260					0.6		
Bromodichloromethane	75-27-4	2.98E-02	1.60E-03	0.0656	-57	1.06E-05	55	0.33	6740	0.08	163.83	2980.734
Bromoform	75-25-2	1.49E-02	5.35E-04	0.021935	8	1.03E-05	87.1	0.5226	3100	0.08	252.75	1942.753
4-Bromophenyl phenyl ether	101-55-3		1.17E-04	0.004797	18.7		17000	102	1.45		249.11	148.0463

Table A4. Chemical Property Values

Chemicals	CAS #	Di cm ² /sec	HLC atm- m ³ /mol	H' unitless	Melting Point (C)	Dw cm ² /sec	Koc cm ³ /g	Kd L/kg	Water Solubility mg/L	GTARC mg/L	Mol. Wt.	Csat mg/kg
Butyl benzyl phthalate	85-68-7	1.74E-02	1.26E-06	5.17E-05	-35	4.83E-06	57500	345	2.69	3	312.37	928.319
Cadmium	7440-43-9				160.5					0.005	112.4	
Captan	133-06-2		7.19E-06	0.000295	178		198	1.188	3.3		300.59	
Carbaryl	63-25-2		1.31E-03	0.05371	142		102	0.612	82.6	0.7	201.23	
Carbazole	86-74-8	3.90E-02	1.53E-08	6.27E-07	246.2	7.03E-06	3390	20.34	7.48		167.21	
Carbofuran	1563-66-2		3.09E-09	1.27E-07	151		48	0.288	32	0.04	221.26	
Carbon disulfide	75-15-0	1.04E-01	3.03E-02	1.24	-115	1.00E-05	45.7	0.2742	1190		76.14	721.2542
Carbon tetrachloride	56-23-5	7.80E-02	3.04E-02	1.25	-23	8.80E-06	174	1.044	793	0.005	153.82	1091.692
Carboxin	5234-68-4		2.80E-01	11.48	94				199	0.7	235.31	
Chloramben	133-90-4		3.87E-07	1.59E-05	200.5		190	1.14	700	0.1	206.3	
Chlordane	12789-03-6	1.18E-02	4.86E-05	0.001993	106	4.37E-06	120000	720	0.056	0.002	409.76	
p-Chloroaniline	106-47-8	4.83E-02	3.31E-07	1.36E-05	72.5	1.01E-05	66.1	0.3966	5300		127.57	
Chlorobenzene	108-90-7	7.30E-02	3.70E-03	0.152	-45.2	8.70E-06	219	1.314	472	0.1	112.56	680.7738
Chloroform	67-66-3	1.04E-01	3.70E-03	0.1517	-63.6	1.00E-05	39.8	0.2388	7920	0.08	119.38	2907.569
2-Chlorophenol	95-57-8	5.01E-02	3.90E-04	0.01599	9.8	9.46E-06	388	2.328	22000	0.04	128.56	53481.67
Chlorothalonil	1897-45-6		2.00E-06	0.000082	250.5		5780	34.68	0.6	0.0015	265.91	
Chlorpyrifos	2921-88-2		2.93E-06	0.00012	41.5		1862	11.172	0.4	0.02	350.59	
Chromium(VI)	18540-29-9				1900			1.90E+01		0.1		
Chrysene	218-01-9	2.48E-02	9.46E-05	3.88E-03	258.2	6.21E-06	3.98E+05		1.60E-03	0.0000044	228.3	
Copper	7440-50-8				1083					1.3	63.5	
Cyanazine	21725-46-2		2.57E-01	10.537	167		200	1.2	170	0.001	240.7	
Cyanide, free	57-12-5							9.90E+00		0.2		
Cyanogen bromide	506-68-3	9.60E-02	5.00E-03	0.205	11.1	1.00E-05	26	0.156	8500		105.93	2501.267
Dalapon, sodium salt	75-99-0		6.43E-08	2.64E-06	-4.4		2.3	0.0138	7430	0.2	142.97	845.5377
2,4-Dichlorophenoxyaceticacid (2,4-D)	94-75-7		1.02E-08	4.18E-07	140.5				677	0.07	221.04	
DDD	72-54-8	1.69E-02	4.00E-06	0.000164	109.5	4.76E-06	1000000	6000	0.09	0.002	320.05	
DDE	72-55-9	1.44E-02	2.10E-05	0.000861	89	5.87E-06	4470000	26820	0.12	0.002	318.03	
DDT	50-29-3	1.37E-02	8.10E-06	0.000332	108.5	4.95E-06	2630000	15780	0.025	0.002	354.49	
Demeton	8065-48-3										258.36	
Diazinon	333-41-5		1.13E-07	4.63E-06			229	1.374	40	0.0006	304.35	58.96003
Dibenz[a,h]anthracene	53-70-3	2.02E-02	1.47E-08	6.03E-07	269.5	5.18E-06	3.80E+06		2.49E-03	0.0000044	278.4	
Dibenzofuran	132-64-9	6.01E-02	2.13E-04	0.008733	86.5	1.00E-05	7760	46.56	4.22		168.2	
1,4-Dibromobenzene	106-37-6		8.93E-04	0.036613	87.31				20		235.92	
Dibromochloromethane	124-48-1	1.96E-02	7.83E-04	0.032103	-20	1.05E-05	63.1	0.3786	2600	0.08	208.29	1259.941
1,2-Dibromo-3-chloropropane	96-12-8	7.00E-06	1.47E-04	0.006027	6	7.00E-06	28	0.168	1230	0.0002	236.34	331.0238
Dibutyl phthalate	84-74-2	4.38E-02	9.38E-10	3.85E-08	-35	7.86E-06	33900	203.4	11.2	2.7	278.35	2279.2
Dicamba	1918-00-9		2.18E-09	8.94E-08	115		115	0.69	4500	0.2	221.04	
1,2-Dichlorobenzene	95-50-1	6.90E-02	1.90E-03	0.0779	-16.7	7.90E-06	617	3.702	156	0.6	147	595.3804

Table A4. Chemical Property Values

Chemicals	CAS #	Di cm ² /sec	HLC atm- m ³ /mol	H' unitless	Melting Point (C)	Dw cm ² /sec	Koc cm ³ /g	Kd L/kg	Water Solubility mg/L	GTARC mg/L	Mol. Wt.	Csat mg/kg
1,4-Dichlorobenzene	106-46-7	6.90E-02	2.43E-03	0.09963	52.7	7.90E-06	617	3.702	73.8	0.075	147	
3,3-Dichlorobenzidine	91-94-1	1.94E-02	4.00E-09	1.64E-07	132.5	6.74E-06	724	4.344	3.11	0.00004	253.13	
1,2-Dichloroethane	107-06-2	1.04E-01	9.79E-04	0.040139	-35.5	9.90E-06	17.4	0.1044	8520	0.005	98.96	1805.325
1,1-Dichloroethylene	75-35-4	9.00E-02	2.61E-02	1.0701	-122.5	1.04E-05	58.9	0.3534	2250	0.007	96.94	1469.592
cis-1,2-Dichloroethylene	156-59-2	7.36E-02	4.08E-03	0.16728	-80	1.13E-05	35.5	0.213	3500	0.07	96.94	1204.79
trans-1,2-Dichloroethylene	156-60-5	7.07E-02	9.38E-03	0.38458	-49.8	1.19E-05	52.5	0.315	6300	0.1	96.94	3066.766
2,4-Dichlorophenol	120-83-2	3.46E-02	3.16E-06	0.00013	45	8.77E-06	147	0.882	4500	0.02	163	
4-(2,4-Dichlorophenoxy) butyric acid (2,4-DB)	94-82-6		2.29E-09	9.39E-08	118		530	3.18	53		249.1	
1,2-Dichloropropane	78-87-5	7.82E-02	2.80E-03	0.1148	-70	8.73E-06	43.7	0.2622	2800	0.005	112.99	1074.162
1,3-Dichloropropene	542-75-6	6.26E-02	1.77E-02	0.7257	-48	1.00E-05	45.7	0.2742	2800	0.0004	110.97	1427.059
Dieldrin	60-57-1	1.25E-02	1.51E-05	0.000619	175.5	4.74E-06	21400	128.4	0.195	0.000002	380.91	
Diethyl phthalate	84-66-2	2.56E-02	4.50E-07	1.85E-05	-40.5	6.35E-06	288	1.728	1080	23	222.24	1974.244
Dimethoate	60-51-5		1.05E-10	4.31E-09	52		27	0.162	23800		229.26	
Dimethyl phthalate	131-11-3		1.05E-07	4.31E-06	0.0		40	0.24	4000	313	194.19	1360.003
2,4-Dimethylphenol	105-67-9	5.84E-02	2.00E-06	0.000082	24.5	8.69E-06	209	1.254	7870	0.54	122.17	10656.1
2,6-Dimethylphenol	576-26-1		6.65E-06	0.000273	45.7		1600	9.6	6050		122.17	
3,4-Dimethylphenol	95-65-8		6.83E-07	2.8E-05	60.8				4760		122.17	
1,3-Dinitrobenzene	99-65-0		3.74E-07	1.53E-05	89.5		106	0.636	53.3	0.001	168.11	
2,4-Dinitrophenol	51-28-5	2.73E-02	4.43E-07	1.82E-05	115	9.06E-06	0.01	0.00006	2790	0.07	184.11	
2,4-Dinitrotoluene	121-14-2	2.03E-01	9.26E-08	3.8E-06	71	7.06E-06	95.5	0.573	270	0.00005	182.14	
2,6-Dinitrotoluene	606-20-2	3.27E-02	7.47E-07	3.06E-05	66	7.26E-06	69.2	0.4152	182	0.00005	182.15	
Di-n-octylphthalate	117-84-0	1.51E-02	6.68E-05	0.002739	-25	3.58E-06	2385	14.31	0.02		390.57	0.28821
Dinoseb	88-85-7		4.56E-07	1.87E-05	40		124	0.744	52	0.007	240.22	
1,4-Dioxane	123-91-1		4.80E-06	0.000197	11.8		17	0.102	1000000	0.003	88.11	202036.7
Diphenamid	957-51-7		3.63E-11	1.49E-09	135				260	0.2	239.32	
Diphenylamine	122-39-4		3.39E-06	0.000139	53.5		600	3.6	53	0.2	169.23	
Diquat	85-00-7		1.42E-13	5.82E-12	337				70800	0.02	344.06	
Disulfoton	298-04-4		3.99E-06	0.000164	-25		1.603	0.009618	16.3	0.0003	274.41	1.787271
Diuron	330-54-1		2.70E-06	0.000111	158.5		380	2.28	42	0.01	233.1	
Endosulfan	115-29-7	1.15E-02	1.12E-05	0.000459	106	4.55E-06	2140	12.84	0.51		406.93	
Endothall	145-73-3		3.62E-15	1.48E-13	144		123	0.738	100000	0.1	186.17	
Endrin	72-20-8	1.25E-02	7.52E-06	0.000308	200	4.74E-06	12300	73.8	0.25	0.002	380.91	
Ethylbenzene	100-41-4	7.50E-02	7.88E-03	0.32308	-94.9	7.80E-06	363	2.178	169	0.7	106.17	395.1741
Ethylene glycol	107-21-1		6.00E-08	2.46E-06	-12.6		4	0.024	1000000	14	62.07	124000.5
Ethylene thiourea	96-45-7		3.08E-10	1.26E-08	203.5		10	0.06	20000	0.0002	102.16	
Fenamiphos	22224-92-6		1.21E-09	4.96E-08	49.2		331	1.986	329	0.002	303.36	
Fluometuron	2164-17-2		1.80E-09	7.38E-08	164		175	1.05	110	0.09	232.21	
Fluoranthene (PAH)	206-44-0	3.02E-02	1.61E-05	0.00066	107.8	6.35E-06	107000	642	0.206	0.3	202.26	

Table A4. Chemical Property Values

Chemicals	CAS #	Di cm ² /sec	HLC atm- m ³ /mol	H' unitless	Melting Point (C)	Dw cm ² /sec	Koc cm ³ /g	Kd L/kg	Water Solubility mg/L	GTARC mg/L	Mol. Wt.	Csat mg/kg
Fluorene (PAH)	86-73-7	3.63E-02	6.36E-05	0.002608	114.8	7.88E-06	13800	82.8	1.98	1.3	166.22	
Fonofos	944-22-9		5.40E-06	0.000221					16	0.01	246.33	
Formaldehyde	50-00-0		3.37E-07	1.38E-05	-92				400000	1	30.03	
Glyphosate	1071-83-6		4.08E-19	1.67E-17	200		3631	21.786	12000	0.7	169.07	
Heptachlor	76-44-8	1.12E-02	1.49E+00	61.008	95.5	5.69E-06	1410000	8460	0.18	0.0004	373.32	
Heptachlor epoxide	1024-57-3	1.32E-02	9.50E-06	0.00039	160	4.23E-06	83200	499.2	0.2	0.0002	389.32	
Hexachlorobenzene	118-74-1	5.42E-02	1.32E-03	0.05412	231.8	5.91E-06	55000	330	6.2	0.001	284.78	
Hexachlorobutadiene	87-68-3	5.61E-02	8.15E-03	0.33415	-21	6.16E-06	53700	322.2	3.23	0.001	260.76	1041.23
a-Hexachlorocyclohexane	319-84-6	1.42E-02	1.06E-05	0.000435	159.5	7.34E-06	1230	7.38	2	0.0000022	290.83	
b-Hexachlorocyclohexane	319-85-7	1.42E-02	7.43E-07	3.05E-05	315	7.34E-06	1260	7.56	0.24	0.0000022	290.83	
g-Hexachlorocyclohexane	58-89-9	1.42E-02	1.40E-05	0.000574	112.5	7.34E-06	1070	6.42	6.8	0.0002	290.83	
d-Hexachlorocyclohexane	319-86-8		4.29E-07	1.76E-05	142		4260	25.56	31.4	0.0000022	290.82	
Hexachlorocyclopentadiene	77-47-4	1.61E-02	2.70E-02	1.107	11.34	7.21E-06	200000	1200	1.8	0.05	272.77	2160.552
Hexachloroethane	67-72-1	2.50E-03	3.89E-03	0.15949	187	6.80E-06	1780	10.68	50	0.001	236.74	
Hexachlorophene	70-30-4		5.48E-13	2.25E-11	164.5		5000	30	140		406.91	
n-Hexane	110-54-3	2.00E-01	1.80E+00	73.8	-95.3	7.77E-06	890	5.34	9.5		86.18	182.552
Hexazinone	51235-04-2		4.11E-13	1.69E-11	116				33000	0.4	252.32	
HMX	2691-41-0		8.67E-10	3.55E-08	276		37	0.222	140	0.4	296.16	45.08
Indeno[1,2,3-cd]pyrene	193-39-5	1.90E-02	1.60E-06	6.56E-05	161.5	5.66E-06	3.47E+06		2.20E-05	0.0000044	276.3	
Isophorone	78-59-1	6.23E-02	6.64E-06	0.000272	-8.1	6.76E-06	46.8	0.2808	12000	0.1	138.21	4570.21
Isopropylbenzene	98-82-8		8.70E-02	3.567	-96		454	2.724	61.3		120.21	213.9272
Lead	7439-92-1									0.015		
Malathion	121-75-5		2.40E-08	9.84E-07	2.85		1797	10.782	143	0.1	330.36	1556.126
Maleic anhydride	108-31-6		3.93E-06	0.000161	52.8				4910		98.06	
Maleic hydrazide	123-33-1	9.00E-02	2.65E-11	1.09E-09	307	1.11E-05	41.5	0.249	6000	4	112.09	
Maneb	12427-38-2		5.64E-07	2.31E-05	200		550	3.3	6		295.37	
Manganese	7439-96-5				682.2					0.05	54.94	
Mercury	7439-97-6	3.07E-02	1.14E-02	0.4674	-39.38	6.30E-06				0.002	401.2	
Methamidophos	10265-92-6		8.68E-11	3.56E-09	44.5				1000000		141.13	
Methanol	67-56-1		4.55E-06	0.000187	-97.68		9	0.054	1000000		32.04	154034.8
Methomyl	16752-77-5	6.93E-02	1.84E-10	7.54E-09	78	1.00E-05	15	0.09	58000	0.2	162.21	
Methoxychlor	72-43-5	1.56E-02	1.58E-05	0.000648	87	4.46E-06	97700	586.2	0.045	0.04	345.66	
2-Methyl-4-chlorophenoxyacetic acid (MCPA)	94-74-6		1.33E-09	5.45E-08	120		89	0.534	1170	0.004	200.62	
Methyl ethyl ketone	78-93-3	8.95E-02	5.69E-05	0.002333	-86	9.80E-06	4.5	0.027	223000		72.11	28418.11
Methyl iodide	74-88-4		5.26E-03	0.21566	-66.45		158	0.948	13900		141.94	15126.77
Methyl isobutyl ketone	108-10-1	7.50E-02	1.38E-04	0.005658	-84	7.80E-06	134	0.804	19000		100.16	17196.07
Methyl parathion	298-00-0		1.00E-07	4.1E-06	35.5		5100	30.6	37.7	0.002	263.21	
2-Methylphenol	95-48-7	7.40E-02	1.20E-06	4.92E-05	29.8	8.30E-06	91.2	0.5472	26000		108.14	16827.44

Table A4. Chemical Property Values

Chemicals	CAS #	Di cm ² /sec	HLC atm- m ³ /mol	H' unitless	Melting Point (C)	Dw cm ² /sec	Koc cm ³ /g	Kd L/kg	Water Solubility mg/L	GTARC mg/L	Mol. Wt.	Csat mg/kg
3-Methylphenol	108-39-4		8.65E-07	3.55E-05	12.22		34.6	0.2076	22700		108.14	6982.67
4-Methylphenol	106-44-5		1.00E-06	0.000041	34.739		49	0.294	21500		108.14	
Methylene chloride	75-09-2	1.01E-01	2.19E-03	0.08979	-95.1	1.17E-05	11.7	0.0702	13000	0.005	84.93	2430.49
Methyl tert butyl ether (MTBE)	1634-04-4		5.87E-04	0.024067	-109		11.2	0.0672	5.10E+04	0.02	88.15	
Metolachlor	51218-45-2		9.00E-09	3.69E-07					530	0.1	283.8	
Metribuzin	21087-64-9		1.81E-12	7.42E-11	126		95	0.57	1220	0.2	214.29	
Mirex	2385-85-5		5.16E-04	0.021156	485		5754	34.524	3.28		545.55	
Molybdenum	7439-98-7				1438.9					0.04	95.94	
Naled	300-76-5		5.00E-07	2.05E-05	27				2000		380.79	
Naphthalene	91-20-3	5.90E-02	4.83E-04	0.019803	80.2	7.50E-06	2000	12	31	0.1	128.18	
Nickel	7440-02-0				790.6					0.1	58.69	
Nitrobenzene	98-95-3	7.60E-02	2.40E-05	0.000984	5.7	8.60E-06	64.6	0.3876	2090	0.017	123.11	1019.468
n-Nitrosodimethylamine	62-75-9		1.82E-06	7.46E-05			12	0.072	1000000	0.0000007	74.08	172013.9
n-Nitrosodiphenylamine	86-30-6	3.12E-02	5.00E-06	0.000205	66.5	6.35E-06	1290	7.74	35.1	0.005	198.23	
Oxamyl	23135-22-0		2.37E-10	9.72E-09	101		8	0.048	280000	0.2	219.26	
Paraquat	4685-14-7		1.00E-09	4.1E-08			15488	92.928	620000	0.03	257.16	57677360
Pendimethalin	40487-42-1		8.56E-07	3.51E-05	57				0.275		281.31	
Pentachlorobenzene	608-93-5		7.10E-04	0.02911	86		40000	240	1.33	0.074	250.34	
Pentachloronitrobenzene	82-68-8		8.00E-05	0.00328	144		26600	159.6	0.55		295.34	
Pentachlorophenol	87-86-5	5.60E-02	2.44E-08	1E-06	174	6.10E-06	592	3.552	1950	0.001	266.34	
Phenol	108-95-2	8.20E-02	3.97E-07	1.63E-05	40.9	9.10E-06	28.8	0.1728	82800	4	94.11	
m-Phenylenediamine	108-45-2		9.53E-11	3.91E-09	62.8				238000		108.14	
Phenylmercuric acetate	62-38-4		5.66E-10	2.32E-08	148.5		67	0.402	4700		336.74	
Phorate	298-02-2		5.76E-06	0.000236	-15		661	3.966	50		260.38	203.3022
Picloram	1918-02-1		4.05E+00	166.05	218.5		26	0.156	430	0.5	241.46	
Polychlorinated biphenyls (PCBs)	1336-36-3		2.83E-04	1.16E-02			3.09E+05		4.30E-02	0.0005	326.44	
Prometon	1610-18-0		1.98E-09	8.12E-08	91.5		525	3.15	750	0.1	225.3	
Pronamide	23950-58-5		1.91E-06	7.83E-05	155.5		200	1.2	15	0.05	256.13	
Propachlor	1918-16-7		1.09E-07	4.47E-06	77		263	1.578	613	0.09	211.69	
Propanil	709-98-8		4.50E-09	1.85E-07	92				225		218.08	
Propazine	139-40-2		4.60E-09	1.89E-07	213		155	0.93	8.6	0.01	229.71	
Propham	122-42-9		3.85E-08	1.58E-06	90		89	0.534	32	0.1	179.22	
n-Propylbenzene	103-65-1	7.50E-02	1.05E-02	0.4305	-99.5	7.80E-06	741	4.446	52.2		120.2	241.496
Pyrene (PAH)	129-00-0	2.72E-02	1.10E-05	0.000451	151.2	7.24E-06	105000	630	0.135	0.96	202.26	
RDX	121-82-4		5.57E-08	2.28E-06	108				933	0.002	172.57	
Rotenone	83-79-4		1.12E-13	4.59E-12	165.5				15		394.43	
Selenium	7782-49-2				217					0.05	78.96	
Silver	7440-22-4				516.6					0.1	107.868	
Silvex	93-72-1		9.06E-09	3.71E-07	181.6		56	0.336	140	0.05	269.51	

Table A4. Chemical Property Values

Chemicals	CAS #	Di cm ² /sec	HLC atm- m ³ /mol	H' unitless	Melting Point (C)	Dw cm ² /sec	Koc cm ³ /g	Kd L/kg	Water Solubility mg/L	GTARC mg/L	Mol. Wt.	Csat mg/kg
Simazine	122-34-9		3.37E-09	1.38E-07	226.5		138	0.828	5.7	0.004	201.66	
Strontium	7440-24-6				769					4		
Strychnine	57-24-9		7.56E-14	3.1E-12	-147.6				160		334.42	
Styrene	100-42-5	7.10E-02	2.75E-03	0.11275	-31	8.00E-06	776	4.656	310	0.1	104.15	1480.884
Terbacil	5902-51-2		1.20E-10	4.92E-09	176		41	0.246	710	0.09	216.67	
Terbufos	13071-79-9		2.40E-05	0.000984	-29.2		661	3.966	5.07	0.0009	288.43	20.61555
1,1,1,2-Tetrachloroethane	630-20-6	7.10E-02	2.42E-03	0.09922	-68.7	7.90E-06	79	0.474	1100	0.07	167.85	651.7732
1,1,2,2-Tetrachloroethane	79-34-5	7.10E-02	3.45E-04	0.014145	-43.8	7.90E-06	93.3	0.5598	2970	0.0003	167.85	1967.448
Tetrachloroethylene	127-18-4	7.20E-02	1.84E-02	0.7544	-22.3	8.20E-06	155	0.93	200	0.005	165.83	234.1643
Tetrahydrofuran	109-99-9		7.05E-05	0.002891	-108.5				1000000		72.11	
Thallium compounds								7.10E+01		0.002	504.8	
Toluene	108-88-3	8.70E-02	6.64E-03	0.27224	-94.9	8.60E-06	182	1.092	526	1	92.14	653.7223
Toxaphene	8001-35-2	1.16E-02	6.00E-06	0.000246	65	4.34E-06	257000	1542	0.74	0.003	413.8	
Triallate	2303-17-5		1.93E-05	0.000791	25		2239	13.434	4		304.67	54.13659
1,2,4-Trichlorobenzene	120-82-1	3.00E-02	1.42E-03	0.05822	17	8.23E-06	1780	10.68	300	0.07	181.45	3237.26
1,3,5-Trichlorobenzene	108-70-3		2.19E-03	0.08979	63.4		708	4.248	6.01	0.04	181.45	
1,1,1-Trichloroethane	71-55-6	7.80E-02	1.72E-02	0.7052	-30.4	8.80E-06	110	0.66	1330	0.2	133.41	1185.878
1,1,2-Trichloroethane	79-00-5	7.80E-02	9.13E-04	0.037433	-36.6	8.80E-06	50.1	0.3006	4420	0.005	133.41	1801.537
Trichloroethylene	79-01-6	7.90E-02	1.03E-02	0.4223	-84.7	9.10E-06	166	0.996	1100	0.005	131.39	1292.312
Trichlorofluoromethane	75-69-4	8.70E-02	9.70E-02	3.977	-110.48	1.30E-05	160	0.96	2050		90.19	3694.865
2,4,5-Trichlorophenol	95-95-4	2.91E-02	4.33E-06	0.000178	69	7.03E-06	1600	9.6	1200	2.6	197.45	
2,4,6-Trichlorophenol	88-06-2	3.18E-02	7.79E-06	0.000319	69	6.25E-06	381	2.286	800	0.003	197.45	
1,2,3-Trichloropropane	96-18-4	7.10E-02	3.43E-04	0.014063	-14.7	7.90E-06	51	0.306	1750	0.04	147.43	715.0939
1,1,2-Trichlorotrifluoroethane	76-13-1	2.88E-02	5.26E-01	21.566	-36.4	8.07E-06	372	2.232	170		187.38	1080.801
Trifluralin	1582-09-8		2.64E-05	0.001082	49		13804	82.824	8.11	0.005	335.29	
1,2,4-Trimethylbenzene	95-63-6	7.50E-02	6.16E-03	0.25256	-43.8	7.10E-06	3720	22.32	57		120.2	1280.627
1,3,5-Trimethylbenzene	108-67-8	7.50E-02	8.77E-03	0.35957	-44.8	7.10E-06	819	4.914	48.2		120.2	244.91
1,3,5-Trinitrobenzene	99-35-4		3.31E-10	1.36E-08	122.5				278		213.11	
2,4,6-Trinitrotoluene	118-96-7		4.57E-07	1.87E-05	80.1		308	1.848	130	0.002	227.13	
Vanadium	7440-62-2				1047						50.94	
Vinyl chloride	75-01-4	1.06E-01	2.70E-02	1.107	-153.7	1.23E-06	18.6	0.1116	2760	0.002	62.5	1154.342
Warfarin	81-81-2		2.77E-09	1.14E-07	161		919	5.514	17		308.34	
White phosphorus	7723-14-0				6.7				3	0.0001	30.97	
Xylenes	1330-20-7	7.00E-02	7.34E-03	0.30094	-47.872	7.80E-06	407	2.442	161	10	106.17	418.3063
Zinc	7440-66-6				215.4					2	65.37	